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Rapports de Recherche

N° 987

Programme 7

PRELIMINARY RESULTS ON AN EXTENSION OF ROE'S APPROXIMATE RIEMANN SOLVER TO NONEQUILIBRIUM FLOWS

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Mars 1989

RR_0987

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Preliminary results on an extension of Roe's approximate Riemann solver to nonequilibrium flows

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PRELIMINARY RESULTS ON AN EXTENSION OF ROE'S RIEMANN SOLVER TO NONEQUILIBRIUM FLOWS

Résultats préliminaires sur une extension du solveur de Riemann de Roe à des écoulements hors équilibre

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Abstract

In this paper, we develop a generalisation of Roe's Riemann solver to the case of a mixture of perfect gases whose equation of state contains vibrational terms. Moreover, we assume that all species are at thermal equilibrium and that the temperatures of translation and vibration are the same.

Then, we develop a semi-implicit scheme for the resolution of 1D problems for flows which are out of the chemical equilibrium. The Riemann solver to be used is the extension of Roe's solver which has been defined at the beginning of this report.

In the last section, some shock tube problems are studied, they show the capacity of this method to solve such problems.

Résumé

Dans ce rapport, nous développons une généralisation du solveur approché de Roe pour le cas de mélanges de gaz parfaits dans lequel l'équation d'état peut contenir des termes de vibration. De plus, nous supposons que les espèces sont à l'équilibre thermique et que les températures de vibration et de translation sont identiques.

Nous développons ensuite un schéma semi-implicite pour le calcul d'écoulements unidimensionnels susceptibles d'être en déséquilibre chimique.

Enfin, ce schéma est testé sur des cas de tubes à choc.

Contents

Notations

- $\mathcal{R}$ is the universal constant of perfect gases
- m_i molar weight of species i
- $R_i = \frac{\mathcal{R}}{m_i}$
- c_{v_i} and c_{p_i} are the specific heats of species i.
- $\gamma_i = \frac{c_{p_i}}{c_{v_i}}$
- $\kappa_i = \gamma_i - 1$
- T is the temperature of the flow
- $\tilde{\gamma}$ is the "sonic gamma", $a^2 = \tilde{\gamma}\,\frac{p}{\rho}$, see Section 2.2, equation (2.8)
- $\tilde{\kappa} = \tilde{\gamma} - 1$, see Section 2.2, equation (2.7)
- ρ_i is the density of species i
- ρ is the total density, $\rho = \sum_{i=1}^{ns} \rho_i$
- $Y_i = \frac{\rho_i}{\rho}$ is the mass fraction of species i
- ${h_i}^0$ is the enthalpy of formation of species i
- θ_i is a typical value of the vibrational temperature of the molecules of species i
- p is the pressure
- u is the velocity, $m = \rho u$ is the momentum
- e is the total energy per unit volume
- ϵ is the specific energy per unit volume
- $H = \frac{e+p}{\rho}$ is the specific enthalpy
- Ω_i is the rate of production of species i

Chapter 1

Introduction

The development of trans-atmospheric vehicule projects has considerably revived research in hypersonic. In particular, many researchers are currently working on the development of numerical schemes for solving the P.D.E. systems which describe the flows around such vehicles.

An important part of these researches is concentrated on the Euler system of equation. The success of TVD schemes (and particularly MUSCL type schemes) to solve them in transonic and supersonic applications gives the legitimate desire of extending these methods to hypersonic design (see [6] and references therein). Here, different phenomena appear, especially chemical ones, due to the high temperature levels which are encountered.

The fundamental tool in a MUSCL scheme is the Riemann solver. One of the most popular is Roe's. Various authors have attempted to generalize it to chemically equilibrium flow (see [5], [13], [11] for example) or to nonequilibrium flow (see [10]).

Several difficulties coming from the integration of the Euler system of equations have been described an analysed in Yee and LeVeque [6], [4].

In this report, we describe a generalisation of Roe's Riemann solver for a mixture of perfect gas with chemical reactions ; our solution is quite different of that of Shuen et al. [10] and uses more deeply the physics of the problem. In particular, Shuen et al. [10] use neither the precise form of the state equation nor the expression of the total energy. This generalisation is the subject of the second part of this report while we give, in the first section, the equations of the system.

In a third part, we develop a semi implicit scheme for the resolution of

1D problem for flows which are out of chemical equilibrium. The Riemann solver to be used is the extension of Roe's solver which has been developed in the second section. The use of the various conservation properties makes the problem much simpler to solve than it might have appeared at first glance.

In a fourth and last part, several shock tube problems are studied, they show the ability of that method to solve such problems.

Chapter 2

Equation of state, Jacobian matrix

2.1 Equation of state

We will consider a mixure of ns perfect gases at thermal equilibrium which interact with each other through a chemical mecanism.

The equation of state is :

$$p = \sum_{i=1}^{ns} \rho_i c_{v_i} \kappa_i T = \rho c_v \kappa T, \tag{2.1}$$

where $c_v = \sum_{i=1}^{ns} Y_i c_{v_i}$ and $\kappa = \dfrac{\sum_{i=1}^{ns} Y_i c_{v_i} \kappa_i}{\sum_{i=1}^{ns} Y_i c_{v_i}}$.

The relation between the temperature, the mass fractions Y_i and the total energy is given by :

$$e = \rho \frac{u^2}{2} + \sum_{i=1}^{ns} \rho_i c_{v_i} T + \sum_{i=1}^{ns} \rho {h_i}^0 + \sum_{i=1}^{ns} \rho_i \frac{R_i \theta_i}{exp\left(\dfrac{\theta_i}{T}\right) - 1}. \tag{2.2}$$

In this equation, the terms $\rho_i \dfrac{R_i \theta_i}{exp\left(\dfrac{\theta_i}{T}\right) - 1}$ are vibrational energy terms. In the case of monoatomic species, they do not exist.

The state variable W

$$W = (\rho_1, \cdots, \rho_{ns}, m, e)^T, \tag{2.3}$$

satisfy the 1-D system of Euler equations for reactive flows which is :

$$\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} = \Omega. \tag{2.4}$$

In 2.4, the flux term is

$$F(W) = \left(\rho_1 u, \cdots, \rho_{ns} u, \rho u^2 + p, u(e+p)\right)^T, \tag{2.5}$$

and the source term Ω is

$$\Omega = (\Omega_1, \cdots, \Omega_{ns}, 0, 0)^T. \tag{2.6}$$

2.2 Computation of the Jacobian matrix

In this paragraph, we give the expression of the Jacobian matrix of the convective part of the Euler equation. For that purpose, we will often denote pressure derivative $\frac{\partial p}{\partial z_i}$ by p_{z_i} where z_i is any of the independant variables of W.

We have :

$$\frac{\partial F}{\partial W} = \begin{pmatrix} (1-Y_1)u & -Y_1 u & \cdots & -Y_{ns} u & Y_1 & 0 \\ -Y_2 u & (1-Y_2)u & \cdots & -Y_2 u & Y_2 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ -Y_{ns} u & -Y_{ns} u & \cdots & (1-Y_{ns})u & Y_{ns} & 0 \\ -u^2 + p_{\rho_1} & -u^2 + p_{\rho_2} & \cdots & -u^2 + p_{\rho_{ns}} & 2u + p_m & p_e \\ (-H + p_{\rho_1})u & (-H + p_{\rho_2})u & \cdots & (-H + p_{\rho_{ns}})u & H + p_m u & (1+p_e)u \end{pmatrix}.$$

We have to get the values of the derivatives of the pressure. We have the following relation (from equation (2.1)) :

$$p_{\rho_i} = c_{v_i} \kappa_i T + \rho c_v \kappa \frac{\partial T}{\partial \rho_i},$$
$$p_m = \rho c_v \kappa \frac{\partial T}{\partial m},$$
$$p_e = \rho c_v \kappa \frac{\partial T}{\partial e}.$$

From the expression of the energy (2.2), we obtain :

$$\rho c_v \frac{\partial T}{\partial \rho_i} = \rho c_v \frac{\frac{u^2}{2} - c_{v_i} T - Z_i - {h_i}^0}{c_v + \sum_{i=1}^{ns} Y_i X_i},$$

$$\rho c_v \frac{\partial T}{\partial m} = -u \left(1 - \frac{\sum_{i=1}^{ns} Y_i X_i}{c_v + \sum_{i=1}^{ns} Y_i X_i} \right),$$

$$\rho c_v \frac{\partial T}{\partial e} = \left(1 - \frac{\sum_{i=1}^{ns} Y_i X_i}{c_v + \sum_{i=1}^{ns} Y_i X_i} \right).$$

In each of these formulas, in order to simplify the writing, we have set :

$$X_i = \frac{R_i {\theta_i}^2}{\left(exp(\frac{\theta_i}{T}) - 1\right)^2},$$

$$Z_i = \frac{R_i \theta_i}{exp(\frac{\theta_i}{T}) - 1}.$$

Hence, we get :

$$p_{\rho_i} = c_{v_i} \kappa_i T + \tilde{\kappa} \left[\frac{u^2}{2} - c_{v_i} T - {h_i}^0 - Z_i \right],$$

$$p_m = -\tilde{\kappa} u,$$

$$p_e = -\tilde{\kappa},$$

where

$$\tilde{\kappa} = \kappa \left[1 - \frac{\sum_{i=1}^{ns} Y_i X_i}{c_v + \sum_{i=1}^{ns} Y_i X_i} \right]. \tag{2.7}$$

To get a complete analogy with what happens in non reactive flow without any vibrational term [16], we shall set :

$$\chi_i = c_{v_i} (\kappa_i - \tilde{\kappa}) T - \tilde{\kappa} {h_i}^0 - \tilde{\kappa} Z_i$$

So, the expression of the derivatives of the pressure p are ;

$$p_{\rho_i} = \chi_i + \tilde{\kappa}\frac{u^2}{2}$$
$$p_m = -\tilde{\kappa}u$$
$$p_e = \tilde{\kappa}$$

This formulation enables us to derive an expression of $\frac{\partial F}{\partial W}$ which is formally identical to the one obtained in [16]. Thus, the sound velocity a is :

$$a^2 = \sum_{i=1}^{ns} Y_i\chi_i + \tilde{\kappa}\left[H - \frac{u^2}{2}\right].$$

In the case we study here, some algebra gives a much simpler expression for a^2 :

$$a^2 = \tilde{\gamma}\frac{p}{\rho} \qquad \text{where} \quad \tilde{\gamma} = \tilde{\kappa} + 1. \tag{2.8}$$

Chapter 3

Computation of the Roe average

3.1 Introduction

Let us recall what the Roe average is for an hyperbolic system of conservation laws with flux function F.

Two states W_L and W_R being given, we seek for a matrix $\bar{A}(W_L, W_R)$ which satisfies the following properties :

1. $F(W_L) - F(W_R) = \bar{A}(W_L, W_R)(W_L - W_R)$;
2. $\bar{A}(W_L, W_R)$ has real eigenvalues and a complete set of eigenvectors ;
3. $\bar{A}(W, W) = A(W)$.

A natural wish is to get an expression with is the same as the one given by Roe in his original paper [14] for a calorically perfect gas. The simplest way to perform this is to seek for an "average" state $\bar{W}$ such that $\bar{A}$ can be written in the form $\bar{A}(W_L, W_R) = A(\bar{W})$. Unfortunately, for complex equations of state, this is probably impossible (Larrouturou et al [2], Liou et al. [11]). Nevertheless, the expression of A shows that its W dependency is expressed through the total enthalpy H, χ_i, κ and the velocity u. So, we will assume the following form for $\bar{A}$:

$$\bar{A} = \begin{pmatrix} (1-\bar{Y}_1)\bar{u} & -\bar{Y}_1\bar{u} & \cdots & -\bar{Y}_{ns}\bar{u} & \bar{Y}_1 & 0 \\ -\bar{Y}_2\bar{u} & (1-\bar{Y}_2)\bar{u} & \cdots & -\bar{Y}_2\bar{u} & \bar{Y}_2 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ -\bar{Y}_{ns}\bar{u} & -\bar{Y}_{ns}\bar{u} & \cdots & (1-\bar{Y}_{ns})\bar{u} & \bar{Y}_{ns} & 0 \\ -\bar{u}^2 + \bar{p_{\rho_1}} & -\bar{u}^2 + \bar{p_{\rho_2}} & \cdots & -\bar{u}^2 + \bar{p_{\rho_{ns}}} & 2\bar{u} - \bar{p_m} & \bar{p_e} \\ (-\bar{H} + \bar{p_{\rho_1}})\bar{u} & (-\bar{H} + \bar{p_{\rho_2}})\bar{u} & \cdots & (-\bar{H} + \bar{p_{\rho_{ns}}})\bar{u} & \bar{H} + \bar{p_m}\bar{u} & (1+\bar{p_e})\bar{u} \end{pmatrix}.$$

where the averaged values of the derivative of the pressure p are defined as :

$$\begin{aligned} \bar{p_{\rho_i}} &= \bar{\chi}_i + \frac{1}{2}\bar{\kappa}\bar{u}^2 \quad for\ i = 1, ns \\ \bar{p_m} &= -\bar{\kappa}\bar{u} \\ \bar{p_e} &= \bar{\kappa} \end{aligned}$$

Hence, it is sufficient to find "averaged" values of H, χ_i, $\tilde{\kappa}$, Y_i and u to define an "averaged" Jacobian matrix.

As we noticed it before, the expression of A is *formally* identical to the one of a non-reactive flow. In [16], the determination of $\bar{u}$, $\bar{Y}_i$ and $\bar{H}$ makes no use of the state equation provided the pressure jump between the two states W_L and W_R obeys the following equation :

$$\Delta p = \sum_{i=1}^{ns} \bar{\chi}_i \Delta\rho_i + \bar{\tilde{\kappa}}\Delta\epsilon \quad \Delta p = p_L - p_R \tag{3.1}$$

If (3.1) is satisfied, we have :

$$\begin{aligned} \bar{u} &= \frac{\sqrt{\rho_R}u_R + \sqrt{\rho_L}u_L}{\sqrt{\rho_R} + \sqrt{\rho_L}} \\ \bar{Y}_i &= \frac{\sqrt{\rho_R}Y_{iR} + \sqrt{\rho_L}Y_{iL}}{\sqrt{\rho_R} + \sqrt{\rho_L}} \\ \bar{H} &= \frac{\sqrt{\rho_R}H_R + \sqrt{\rho_L}H_L}{\sqrt{\rho_R} + \sqrt{\rho_L}} \end{aligned} \tag{3.2}$$

Now, we have to find expressions for $\bar{\chi}_i$ and $\bar{\tilde{\kappa}}$ which satisfy (3.1).
In these calculations, we will use the operator Δ which is defined by :

Given two states f_R and f_L of a real function f of the variable W,
$$\Delta f = f_L - f_R.$$

let us recall some rules of computation for the Δ operator.

If we use the following notations :

$$\bar{a} = \frac{\sqrt{\rho_R}a_R + \sqrt{\rho_L}a_L}{\sqrt{\rho_R} + \sqrt{\rho_L}} \tag{3.3}$$

$$\underline{a} = \frac{\sqrt{\rho_R}a_L + \sqrt{\rho_L}a_R}{\sqrt{\rho_R} + \sqrt{\rho_L}}, \tag{3.4}$$

we have :

$$\Delta(ab) = \underline{a}\Delta b + \bar{b}\Delta a$$
$$\underline{\rho a} = \underline{\rho}\bar{a}$$

3.2 Determination of $\bar{\bar{\kappa}}$ and $\bar{\chi}_i$

Until they are fully specified, the values of $\bar{\chi}_i$ and $\bar{\bar{\kappa}}$ will be denoted by $\tilde{\chi}_i$ and $\tilde{\bar{\kappa}}$.

We will assume that $\tilde{\chi}_i$ can be written as :

$$\tilde{\chi}_i = c_{v_i}(\kappa_i - \tilde{\bar{\kappa}})\tilde{T} - \tilde{\bar{\kappa}}{h_i}^0 - \tilde{\bar{\kappa}}\tilde{Z}_i \tag{3.5}$$

We have then to find expressions of $\tilde{\bar{\kappa}}$, $\tilde{T}$ and $\tilde{Z}_i$ such that (3.1) holds :

$$\begin{aligned} \textstyle\sum_{i=1}^{ns} \Delta(\rho_i c_{v_i}\kappa_i T) &= \textstyle\sum_{i=1}^{ns} \left(c_{v_i}[\kappa_i - \tilde{\bar{\kappa}}]\tilde{T}\Delta\rho_i - \tilde{\bar{\kappa}}{h_i}^0\Delta\rho_i - \tilde{\bar{\kappa}}\tilde{Z}_i\Delta\rho_i\right] \\ &+ \textstyle\sum_{i=1}^{ns} \tilde{\bar{\kappa}}\left[\Delta(\rho_i c_{v_i}T) + {h_i}^0\Delta\rho_i + \Delta(\rho_i Z_i)\right] \end{aligned} \tag{3.6}$$

The right-hand side of (3.6) is :

$$\sum_{i=1}^{ns} c_{v_i}\kappa_i\tilde{T}\Delta\rho_i + \tilde{\bar{\kappa}}\left[\Delta(\rho_i c_{v_i}T) - c_{v_i}\tilde{T}\Delta\rho_i\right] + \tilde{\bar{\kappa}}\left[\Delta(\rho_i Z_i) - \tilde{Z}_i\Delta\rho_i\right]$$

(There is no more ${h_i}^0$ terms).

It is natural to set $\tilde{Z}_i = \overline{Z}_i$ and $\tilde{T} = \overline{T}$ since :

$$\Delta(\rho_i T) - \bar{T}\Delta\rho_i = \underline{\rho_i}\Delta T$$
$$\Delta(\rho_i Z_i) - \overline{Z}_i\Delta\rho_i = \underline{\rho_i}\Delta Z_i$$

Then, (3.6) becomes :

$$\sum_{i=1}^{ns}\left(c_{v_i}\kappa_i\overline{T}\Delta\rho_i + \tilde{\bar{\kappa}}c_{v_i}\underline{\rho_i}\Delta T + \tilde{\bar{\kappa}}\underline{\rho_i}\Delta Z_i\right) = \sum_{i=1}^{ns}\Delta(\rho_i c_{v_i}\kappa_i T)$$

Since

$$\Delta(\rho_i c_{v_i}\kappa_i T) = \underline{\rho_i}c_{v_i}\kappa_i\Delta T + \overline{T}c_{v_i}\kappa_i\Delta\rho_i,$$

this is equivalent to

$$\underline{\rho\overline{c_v}}\ \overline{\kappa}\Delta T = \tilde{\bar{\kappa}}\left[\underline{\rho\overline{c_v}}\Delta T + \sum_{i=1}^{ns}\underline{\rho_i}\Delta Z_i\right]$$

where we have $\overline{c_v} = \sum_{i=1}^{ns}\overline{Y}_i c_{v_i}$ and

$$\overline{\kappa} = \frac{\sum_{i=1}^{ns}\overline{Y}_i c_{v_i}\kappa_i}{\sum_{i=1}^{ns}\overline{Y}_i c_{v_i}}.$$

If $\Delta T \neq 0$, for this last equality to be satisfied, we set :

$$\tilde{\bar{\kappa}} = \frac{\overline{c_v}\ \overline{\kappa}\Delta T}{\overline{c_v}\Delta T + \sum_{i=1}^{ns}\overline{Y}_i\Delta Z_i}.$$

If $\Delta T = 0$, we will have :

$$\tilde{\bar{\kappa}} = \frac{\bar{c}_v\bar{\kappa}}{\bar{c}_v + \sum_{i=1}^{ns}\bar{Y}_i X_i}. \tag{3.7}$$

Some comments :

- The X_i's depend only on T and are monotone increasing functions. The denominators in (3.2) and (3.7) never vanish ; hence, the definition of $\tilde{\bar{\kappa}}$ is always valid.

- The calculation which have been done in this section does not use the precise form of the internal energy per unit volume. The only assumptions which are really used are the following ones:

  1. The mixture of gases is at thermal equilibrium
  2. It obeys the following law :
     - we assume the pressure is written as :

$$p = \sum_{i=1}^{ns} \rho_i g_i(T)$$

       where the g_i's are monotone increasing functions of the temperature.
     - The internal energy has the following form :

$$\epsilon = \sum_{i=1}^{ns} \rho_i f_i(T)$$

       where the f_i's are monotone increasing functions of the temperature.

It that case, the expression we have given for the Roe average of A can be extended in a straightforward manner. Equations (3.2) are still valid, the expressions of $\bar{\bar{\kappa}}$ and $\bar{\chi}_i$ are the following ones:

$$\bar{\bar{\kappa}} = \frac{\sum_{i=1}^{ns} \bar{Y}_i \Delta f_i}{\sum_{i=1}^{ns} \bar{Y}_i \Delta g_i} .$$

$$\bar{\chi}_i = \bar{g}_i{}' - \bar{\bar{\kappa}} \bar{f}_i$$

Chapter 4

A semi-implicit numerical scheme for the Euler equation with source terms

4.1 Introduction

To begin, let us recall the system of conservation laws we intend to solve numerically. If we set

$$W = (\rho_1, \cdots, \rho_{ns}, \rho u, e) \tag{4.1}$$

$$F(W) = \left(\rho_1 u, \cdots, \rho_{ns} u, \rho u^2 + p, u(e+p)\right) \tag{4.2}$$

$$\Omega = (\Omega_1, \cdots, \Omega_{ns}, 0, 0) \tag{4.3}$$

we have

$$\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} = \Omega \tag{4.4}$$

From a mathematical point of view, the systems we are interested in are those where the Jacobian matrix of Ω with respect to W have eigenvalues with a negative real part. We shall assume this is true for air though there are no theoretical evidence of this, as far as we know.

4.2 First order scheme, analysis

The scheme is explicit for the convective terms and implicit for the source terms.

$$W_j^{n+1} - W_j^n = \lambda \left(\mathcal{F}(W^n{}_{j+1}, W_j^n) - \mathcal{F}(W_j^n, W^{n-1}{}_{j-1}) \right) + \Delta t \ \Omega(W_j^{n+1}) \tag{4.5}$$

where $\mathcal{F}$ is the numerical flux which will be the extension of Roe's Riemann solver defined in the previous section. In 4.5, λ is the ratio of the time step over the local mesh size.

To make (4.5) easier to solve, we linearize the Ω term. Hence, we get :

$$\left(I - \Delta t \frac{\partial \Omega}{\partial W}(W_j^n) \right) \delta W_j = \lambda (\mathcal{F}(W_{j+1}{}^n, W_j^n) - \mathcal{F}(W_j^n, W_{j-1}{}^n)) + \Delta t \Omega(W_j^n) \tag{4.6}$$

This is a $(ns+2) \times (ns+2)$ system. In fact, (4.6) is much simpler to solve due to the form of Ω and to some conservation relations as it will be explained now in a very general context and in the next paragraph on the example of a model for air.

The term Ω has no influence on the evolution of momentum and energy. Hence, the evolution of energy and momentum can be computed as for the explicit scheme without any source terms.

Moreover, the continuous system (4.6) has the property of conserving the local proportion of atoms of any element. This is translated through relations of the type :

$$\alpha_k \sum_{i=1}^{ns} a_i{}^1 \frac{\rho_i}{m_i} = \beta_k \sum_{i=1}^{ns} a_i{}^k \frac{\rho_i}{m_i} \qquad k = 2, na \tag{4.7}$$

where na is the number of type of atoms in the mixture and (α_k, β_k) are constants translating the local proportion of atoms of type 1 versus those of type k.

An important assumption to make at this level is to assume that these proportions are uniform in the domain of computation. (We assume here that there is no diffusion at all.) This is true for reentry problems and related phenomena (for example, hypersonic nozzles).

For example, let us consider the chemical reaction :

$$O_2 + N_2 \rightleftharpoons 2NO \tag{4.8}$$

If m_{O_2} (resp. m_{N_2}, m_{NO}) is the molar weight of diatomic oxygen (resp. diatomic nitrogen, and NO), if ρ_{O_2} (resp. ρ_{N_2}, ρ_{NO}) is the density of diatomic oxygen (resp. of nitrogen and NO), then the number of mole of oxygen per unit volume is :

$$\frac{\rho_{O_2}}{m_{O_2}} + \frac{\rho_{NO}}{m_{NO}}$$

and that of nitrogen is :

$$\frac{\rho_{O_2}}{m_{O_2}} + \frac{\rho_{NO}}{m_{NO}}.$$

The reaction (4.8) cannot change both numbers of mole, hence their ratio. So, we have :

$$\frac{\rho_{O_2}}{m_{O_2}} + \frac{\rho_{NO}}{m_{NO}} = \alpha \left(\frac{\rho_{O_2}}{m_{O_2}} + \frac{\rho_{NO}}{m_{NO}} \right),$$

where α is constant in time.

One should expect that scheme (4.6) satisfies this property. In appendix A, we indeed show that the Roe's Riemann solver defined in the previous section has the property of conserving the local proportion of atoms. Moreover, the source terms Ω_i satisfy the relations :

$$\sum_{i=1}^{ns} {a_i}^k \frac{\Omega_i}{m_i} = 0 \qquad k = 1, na \tag{4.9}$$

since there is no production of atoms (no nuclear reactions !). Statement (4.9) implies :

$$\sum_{i=1}^{ns} \frac{{a_i}^k}{m_i} \frac{\partial \Omega_i}{\partial \rho_l} = 0 \tag{4.10}$$

for any $l \geq 1$. Hence, the following relations are true for (4.5).

$$\sum_{i=1}^{ns} \frac{{a_i}^k}{m_i} \delta\rho_i = \sum_{i=1}^{ns} \frac{{a_i}^k}{m_i} RHS_i \tag{4.11}$$

Here, RHS_i is the i^{th} component of the right hand side of (4.6). Due to (4.9) and (4.10), the right-hand side of (4.11) **does not** contain any Ω_i terms ; only flux terms are involved. Hence a lot of computing time is saved.

4.3 Numerical resolution, example

To enlighten what we said before, let us give an example. We will consider a mixture of diatomic oxygen O_2, diatomic nitrogen N_2 monoatomic oxygen O and nitrogen N and NO. The chemical reaction model will be that of Park [3] and has been extensively used in [8]. The local proportion of oxygen versus that of nitrogen is everywhere $\frac{21}{79}$. In the sequel, the subscript 1 (resp. 2, 3, 4, 5) will denote monoatomic oxygen (O) (resp. N, NO, O_2, N_2).Under these conditions, (4.5) becomes :

$$A\,(\delta\rho_1, \delta\rho_2, \ldots, \delta\rho_5, \delta m, \delta e)^T = (RHS_1, \ldots, RHS_7)^T \tag{4.12}$$

$$\frac{\delta\rho_1}{m_1} + \frac{\delta\rho_3}{m_3} + 2\,\frac{\delta\rho_4}{m_4} = \frac{RHS_1}{m_1} + \frac{RHS_3}{m_3} + 2\,\frac{RHS_4}{m_4} \equiv \mathcal{B} \tag{4.13}$$

$$\frac{\delta\rho_2}{m_2} + \frac{\delta\rho_3}{m_3} + 2\,\frac{\delta\rho_5}{m_5} = \frac{RHS_2}{m_2} + \frac{RHS_3}{m_3} + 2\,\frac{RHS_5}{m_5} \equiv \mathcal{C} \tag{4.14}$$

The matrix A in (4.12) is :

$$A = I - \Delta t \begin{pmatrix} \frac{\partial\Omega_1}{\partial\rho_1} & \cdots & \frac{\partial\Omega_1}{\partial\rho_5} & \frac{\partial\Omega_1}{\partial m} & \frac{\partial\Omega_1}{\partial e} \\ \frac{\partial\Omega_2}{\partial\rho_1} & \cdots & \frac{\partial\Omega_2}{\partial\rho_5} & \frac{\partial\Omega_2}{\partial m} & \frac{\partial\Omega_2}{\partial e} \\ \frac{\partial\Omega_3}{\partial\rho_1} & \cdots & \frac{\partial\Omega_3}{\partial\rho_5} & \frac{\partial\Omega_3}{\partial m} & \frac{\partial\Omega_3}{\partial e} \end{pmatrix} \tag{4.15}$$

and

$$(RHS_i) = \lambda\,[\mathcal{F}({W_{j+1}}^n, {W_{j1}}^n) - \mathcal{F}({W_j}^n, {W_{j-1}}^n)] + \Delta t\;\Omega({W_j}^n) \qquad for\ i = 1, 7 \tag{4.16}$$

Let us recall that (4.13) and (4.14) make no use of the source terms despite the presence of Ω terms in (4.16).

From (4.15) and (4.16), since $m_4 = 2m_1$ and $m_5 = 2m_2$, we get

$$\delta\rho_4 = m_1\mathcal{B} - \frac{m_1}{m_3}\delta\rho_3 - \delta\rho_1$$

$$\delta\rho_5 = m_1\mathcal{C} - \frac{m_2}{m_3}\delta\rho_3 - \delta\rho_2$$

So, (4.12) becomes

$$\left(I - \Delta t A'\right)(\delta\rho_1, \delta\rho_2, \delta\rho_3)^T = RHS'$$

where

$$A' = \begin{pmatrix} \frac{\partial\Omega_1}{\partial\rho_1} - \frac{\partial\Omega_1}{\partial\rho_4} & \frac{\partial\Omega_1}{\partial\rho_2} - \frac{\partial\Omega_1}{\partial\rho_5} & \frac{\partial\Omega_1}{\partial\rho_3} - \frac{m_1}{m_3}\frac{\partial\Omega_1}{\partial\rho_4} - \frac{m_2}{m_3}\frac{\partial\Omega_1}{\partial\rho_5} \\ \frac{\partial\Omega_2}{\partial\rho_1} - \frac{\partial\Omega_2}{\partial\rho_4} & \frac{\partial\Omega_2}{\partial\rho_2} - \frac{\partial\Omega_2}{\partial\rho_5} & \frac{\partial\Omega_2}{\partial\rho_3} - \frac{m_1}{m_3}\frac{\partial\Omega_2}{\partial\rho_4} - \frac{m_2}{m_3}\frac{\partial\Omega_2}{\partial\rho_5} \\ \frac{\partial\Omega_3}{\partial\rho_1} - \frac{\partial\Omega_3}{\partial\rho_4} & \frac{\partial\Omega_3}{\partial\rho_2} - \frac{\partial\Omega_3}{\partial\rho_5} & \frac{\partial\Omega_3}{\partial\rho_3} - \frac{m_1}{m_3}\frac{\partial\Omega_3}{\partial\rho_4} - \frac{m_2}{m_3}\frac{\partial\Omega_3}{\partial\rho_5} \end{pmatrix}$$

and

$$RHS' = (RHS)_{i=1,3} + \Delta t \left(\frac{\partial\Omega_i}{\partial m}\delta m + \frac{\partial\Omega_i}{\partial e}\delta e + m_1\frac{\partial\Omega_i}{\partial\rho_4}\mathcal{B} + m_2\frac{\partial\Omega_i}{\partial\rho_5}\mathcal{C}\right)_{i=1,3}$$

Thus, the resolution of (4.6) has been reduced to the resolution of a 3×3 system of linear equations.

Chapter 5

Numerical results

To validate the Riemann solver we propose several numerical tests chosen from Montagné [9]. They are defined as follows :

		Density kg/m^3	Pressure N/m^2	Temp. K	Energy $(m/sec)^2$	Velocity m/sec	Mach
Case A	left	.066	$9.84\ 10^4$	4390	$7.22\ 10^6$	0	0
	right	0.03	$1.50\ 10^4$	1378	$1.44\ 10^6$	0	0
Case B	left	1.00	$6.50\ 10^5$	2242	$2.00\ 10^6$	0	0
	right	0.01	$1.00\ 10^3$	346	$2.50\ 10^5$	0	0
Case C	left	.010	$5.73\ 10^2$	199	$1.44\ 10^5$	4100	14.4
	right	.010	$5.73\ 10^2$	199	$1.44\ 10^5$	−4100	−14.4

Case A is a shock tube with a moderate density and energy ratio. The resulting shock wave is of moderate strength but significant real gas effects are found in this temperature range. Case B is a shock tube with very large density and energy ratios, it produces a large transonic expansion wave. Case C is a Riemann problem with equal and oppositely directed velocities, and the same thermodynamical state on both sides. It produces two strong shocks moving in opposite directions, the temperature increases rapidely so that very important real gas effects occur. In each case, the initial distribution of mass fraction was obtained assuming chemical equilibrium [3].

For each case, we present the density, the velocity, the Mach number, the temperature and the mass fraction profiles of each of the five species.

To obtain a second-order approximation, we use a predictor-corrector method. A linear distribution is introduced in each cell, as usually . To avoid

artificial oscillations, a slope limiting procedure is applied on characteristic fields. The minmod limiter was applied on fields $u - a$ and $u + a$ while superbee limiter was used on the fields corresponding to the u eigenvalue. (for all these problems, see Van Leer [15] for example).

It can be seen by on Figures 5.1 and 5.2, that the method does improve the results especially in expansion and shock waves. The results are better in the contact discontinuity though the solution spreads on several points.

We use Park's model [3], the expression of Ω are taken form his work. Experimental results have shown that :

- The eigenvalues of $\frac{\partial \Omega}{\partial W}$ have negative real parts,
- The maximum time step which can be used in practice is of the order of 0.2. Its value is still dictated by the stiffness of the source term. A more detailled discussion of the choice of the time step can be found in Désideri et al. [7]

The shock tube is taken to be 1 meter long, the mesh is regular. For case A and B, we used 100 grid points. For case B, we used several meshes. The results which are presented used 100 and 500 grid points.

On Figure 5.4 (case A), one can observe a large jump in temperature at the contact discontinuity which varies from about 1200 K (where no chemical reaction occurs) to about 4600 K. The discontinuity is handled without any oscillation. In the contact discontinuity, pressure and the velocity remain constant as they should.

Figures 5.5, 5.7 and 5.8 correspond to case B. In this case, important non equilibrium effects are encountered as can be seen on Figure 5.5. Here, the mass fractions of each of the species do not remain constant between the expansion wave and the contact discontinuity (where a large jump in temperature is encountered). This has a physical explanation : the fluid particles which are close to the contact discontinuity have not the same history than those which are close to the end of the expansion wave. They had to face a more violent phenomenon and had more time to relax. Moreover, one can see that N, O have not the same behaviour as NO, O_2 and N_2, The latter species have a frozen-like behaviour. This is confirmed by a 500 points simulation (Figure 5.6). What is not clear here is the behaviour of O after the contact discontinuity : is there no more monoatomic oxygen or is there a relaxation

phenomenon ? We have the same question with N : is the origin of the small bump in N at the contact discontinuity purely numerical or not ?

A similar phenomena occurs for a flow around a wedge [12]. The fluid particles that are close of the edge remains in an approximately frozen state. They had not time "to see what was happening". Those which are in the expansion wave and are far from the edge are in thermodynamical states that depend on their location.

Figures 5.9, 5.10 and 5.11 correspond to case C. The variation of the mass fraction just behind the shock wave seems to be physically relevant. We ran this experiment with different resolutions (100, 200 and 400 grid points) and different time steps. The results look always the same ; in particular, the maxima just behind the shock wave always have the same magnitude. Similar results were obtained behind a stationary shock wave by Désideri et al. [7] or Brun et al. [17]. Similar behaviours are also described in Zel'dovich et al. [1]

On the contrary, the oscillation in the location of the discontinuity at initial time is of numerical origin.

Conclusion

In this report, we studied the Euler system of equation for the flow of a gas which is a mixture of several perfect gas in which chemical reactions occur. For that purpose, we developed a Roe average formula for the convective part of the Euler equations and a semi-implicit scheme for solving the whole system of equations. We believe that our solution for The Roe average is more consistent with the physic involved by the Euler system of Equation than that Shuen et al. [10].

The solution of the linear system of equation resulting from the semi-implicit scheme is simplified by the use of conservation relations. Hence we got a much simpler system to solve.

The numerical tests we performed show the capacity of this scheme to handle very large discontinuities. Nevertheless, it is necessary to improve it both for robustness and efficiency, since the CFL numbers that can be used are of the order of 0.2.

Acknowledgements : I wish to acknowledge my colleagues more particularily J.L. Montagné for inspiring this work and ONERA where parts of this work were done, L. Fezoui, A. Dervieux, J.A. Désidéri, B. Larrouturou for helpful comments (and carefull reading of the manuscript) and N. Glinsky and E. Hettena for providing me with the first versions of my chemistry Fortran subroutines.

Figures

Figure 5.1: Partial and total densities for case A, first-order calculation

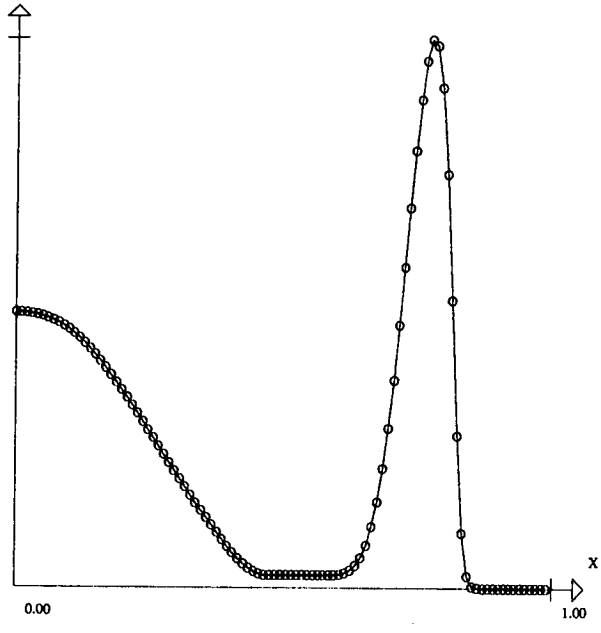


Figure 5.2: Partial and total densities for case A, second-order calculation

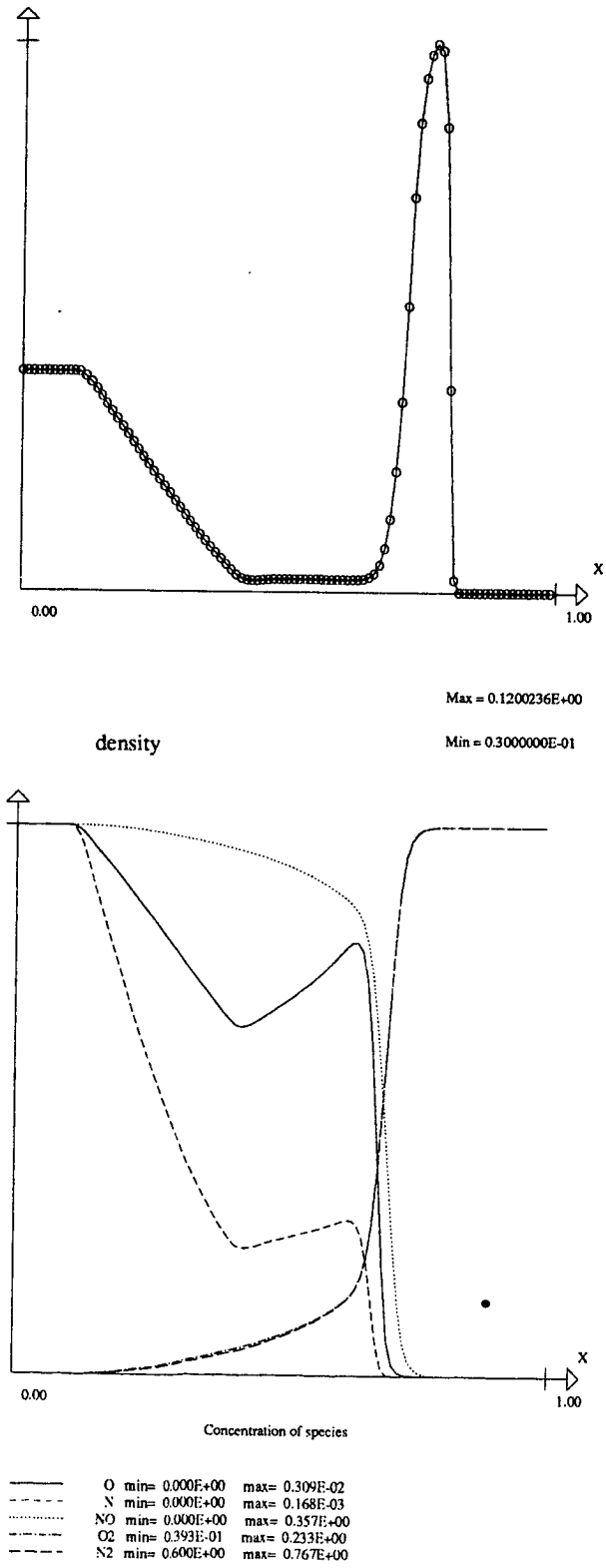
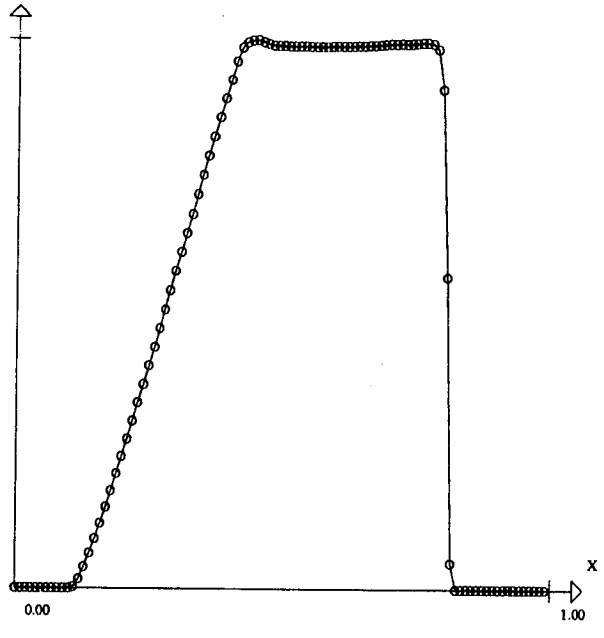


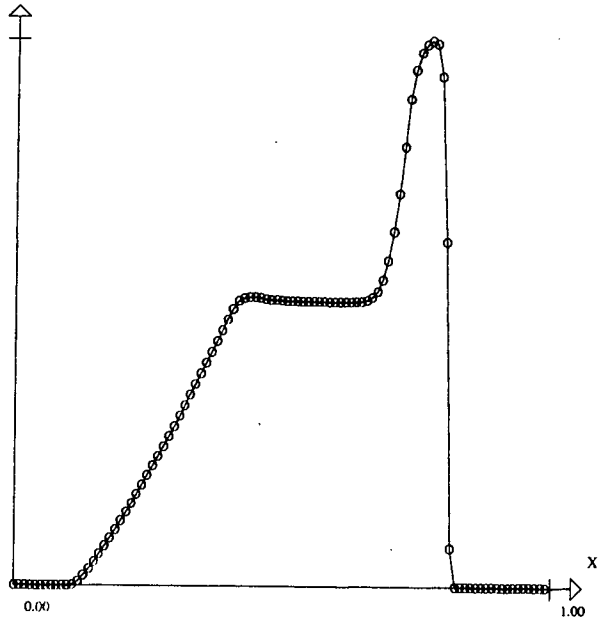
Figure 5.3: Velocity and Mach number for case A, second-order calculation



Max = 0.1066264E+04

Min =-0.1074857E-09

velocity

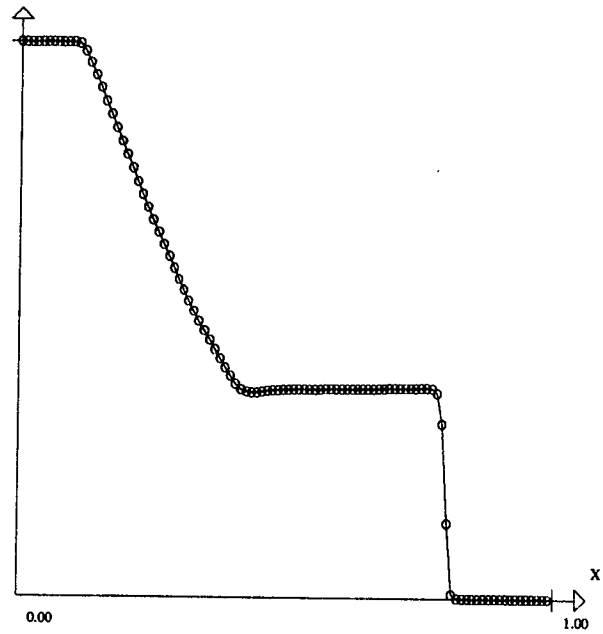


Max = 0.1435614E+01

Min = 0.0000000E+00

Mach

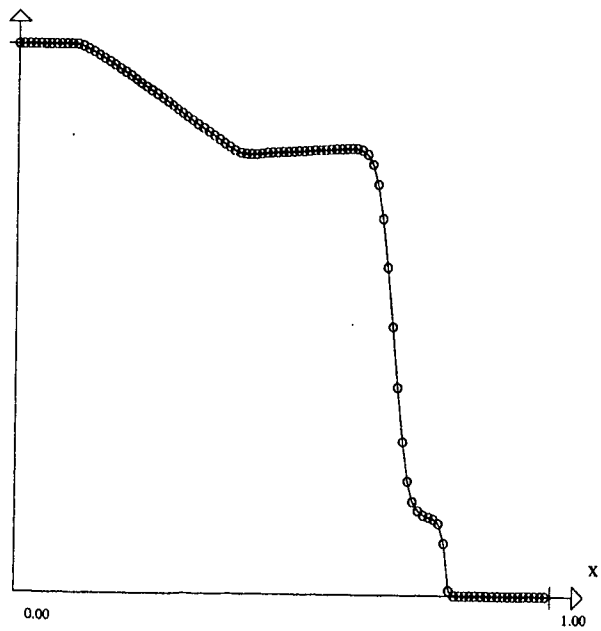
Figure 5.4: Pressure and temperature for case A, second-order calculation



Max = 0.1232642E+06

Min = 0.5206802E+04

pressure

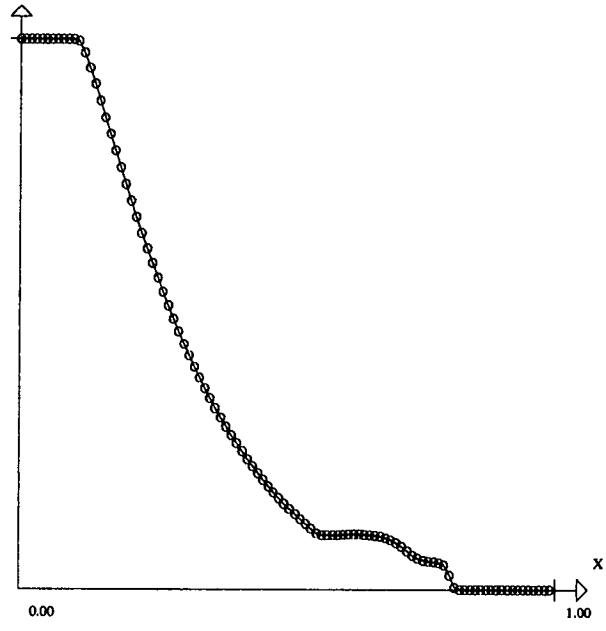


Max = 0.6459147E+04

Min = 0.6020244E+03

temperature

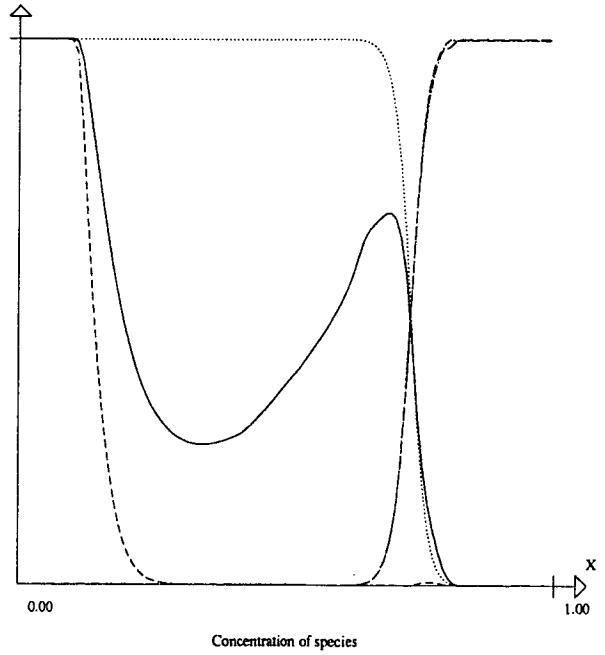
Figure 5.5: Partial and total densities for case B, second-order calculation, mesh with 100 points



Max = 0.1000000E+01

Min = 0.9999999E-02

density



Concentration of species

O min= 0.000E+00 max= 0.517E-06
N min= 0.000E+00 max= 0.861E-12
NO min= 0.000E+00 max= 0.170E-01
O2 min= 0.224E+00 max= 0.233E+00
N2 min= 0.759E+00 max= 0.767E+00

Figure 5.6: Partial and total densities for case B, second-order calculation, mesh with 500 points

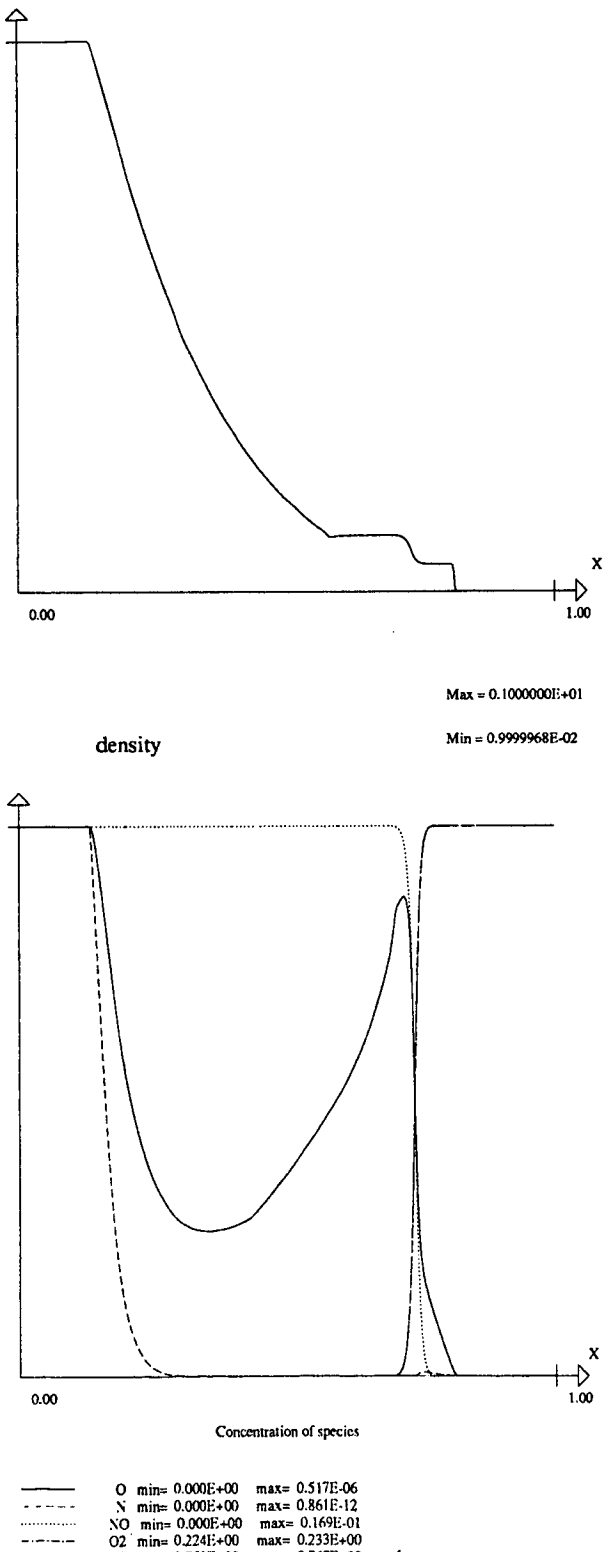


Figure 5.7: Velocity and Mach number for case B, second-order calculation

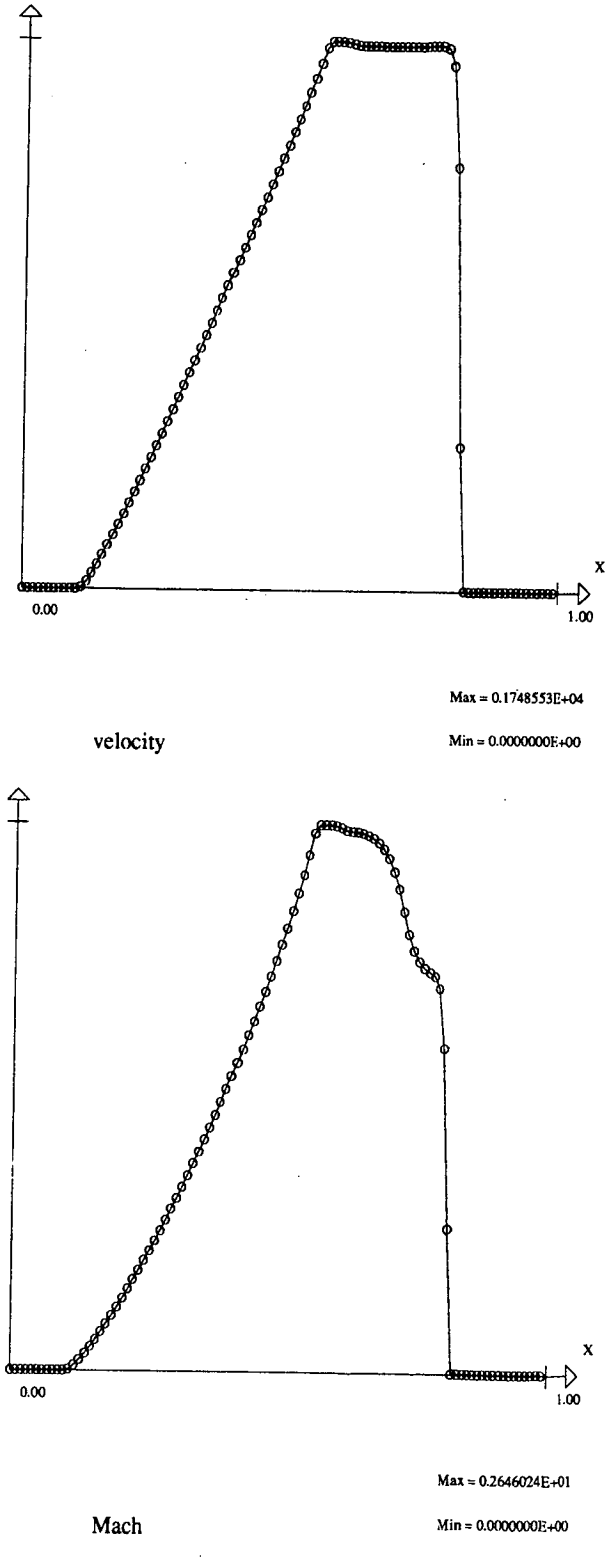


Figure 5.8: Pressure and temperature number for case B, second-order calculation

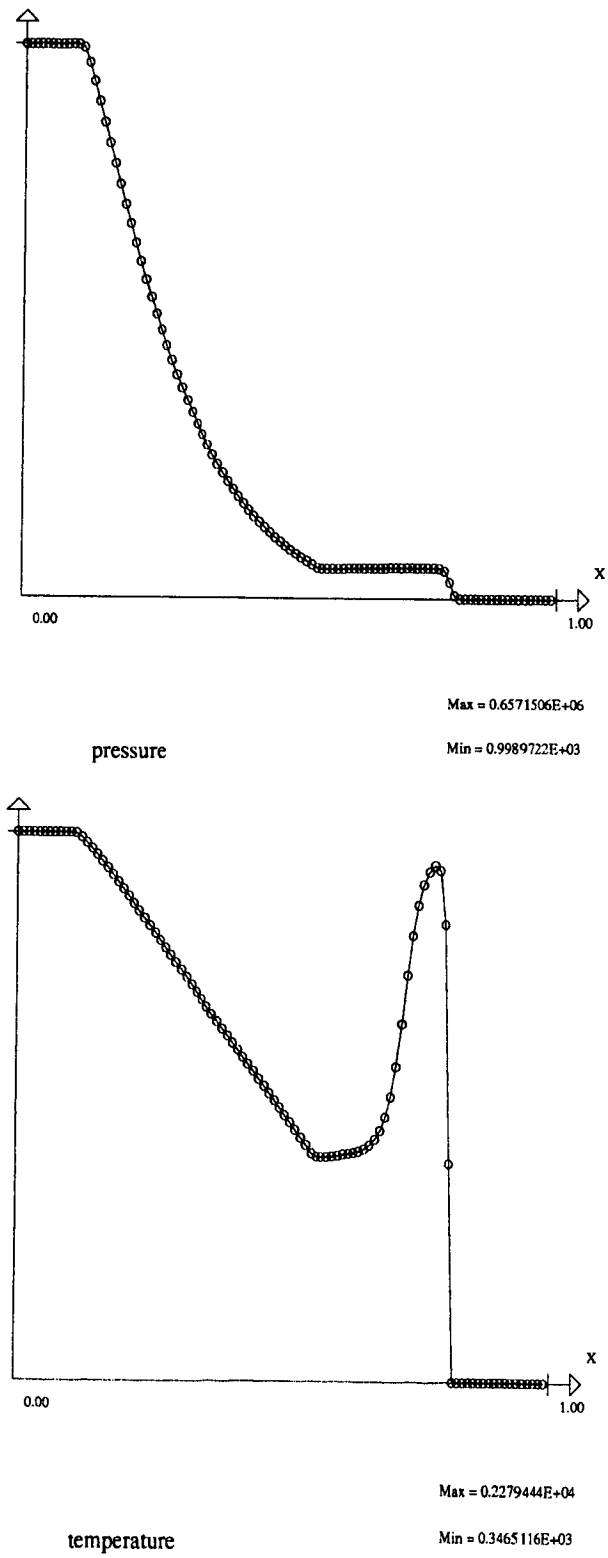


Figure 5.9: Partial and total densities for case C, first-order calculation

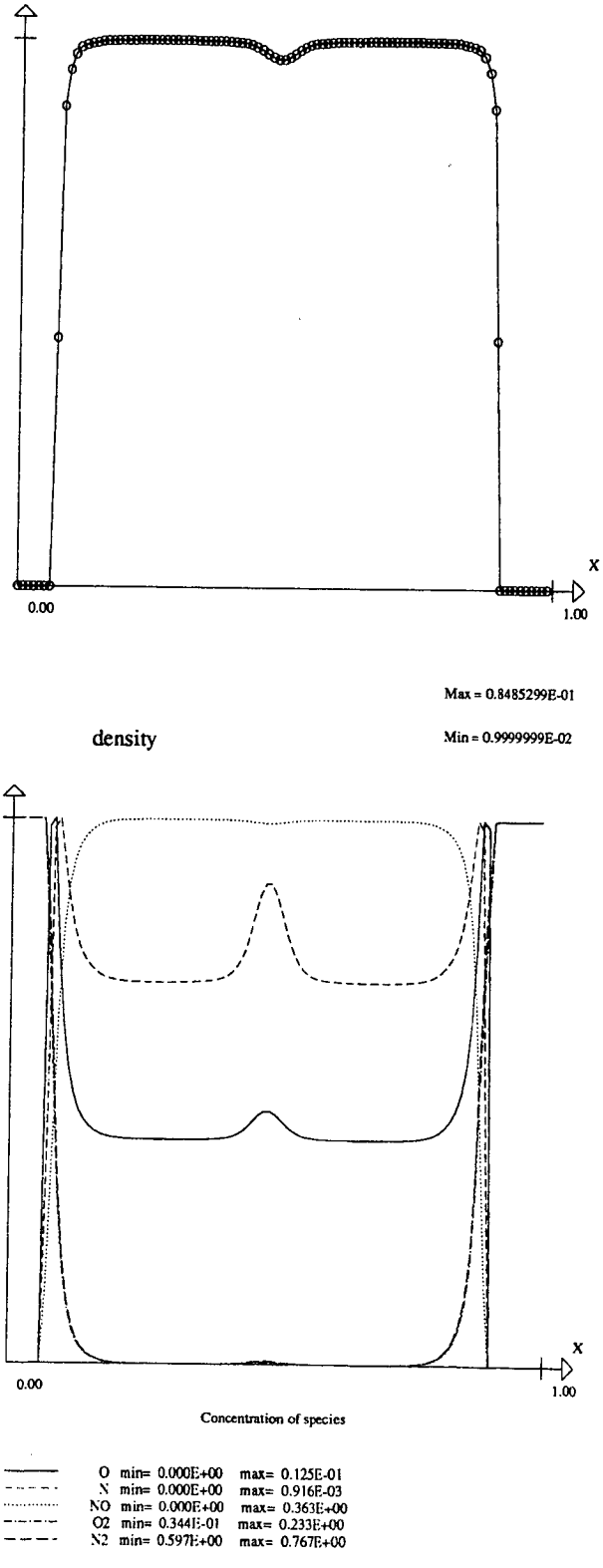
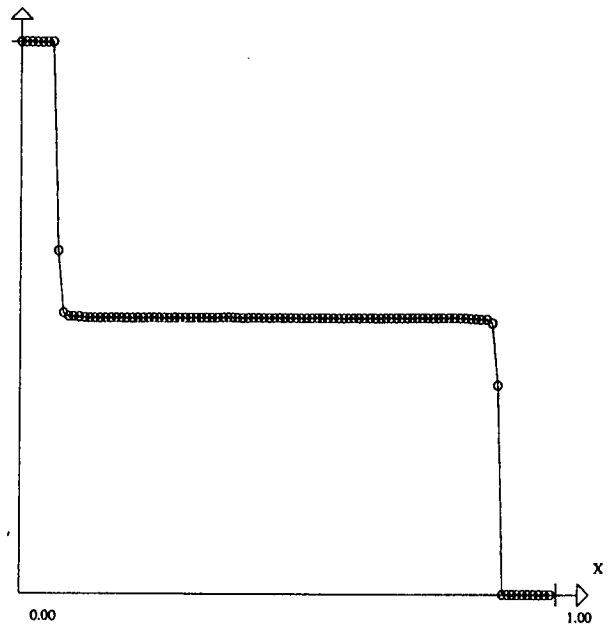


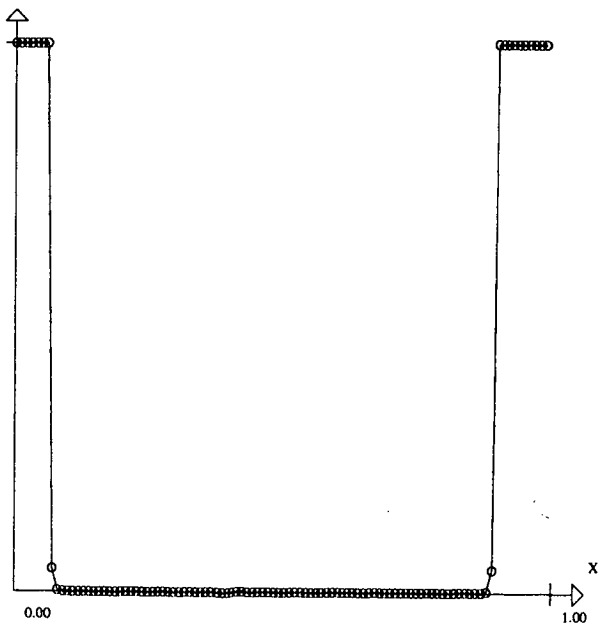
Figure 5.10: Velocity and Mach number for case C, first-order calculation



Max = 0.4100000E+04

velocity

Min =-0.4100000E+04

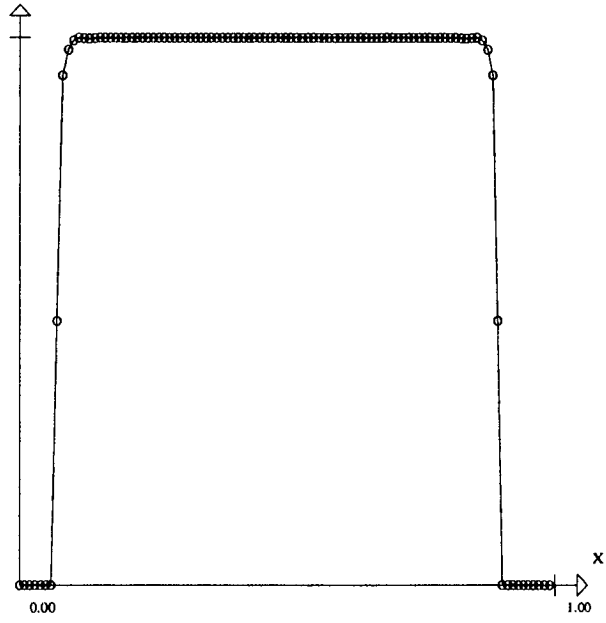


Max = 0.1443845E+02

Mach

Min = 0.7178664E-07

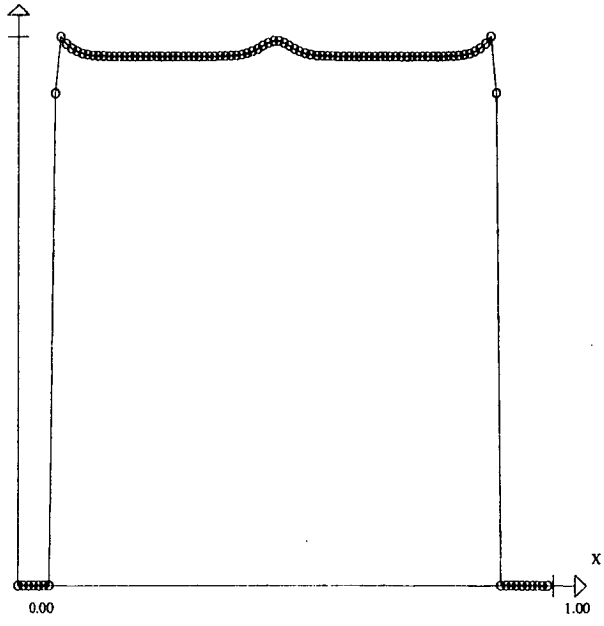
Figure 5.11: Pressure and temperature number for case C, first-order calculation



Max = 0.1911336E+06

Min = 0.5759925E+03

pressure



Max = 0.8054420E+04

Min = 0.1997934E+03

temperature

Appendix A

Conservation of the local proportion of atoms

The question we will answer here is the following : does Scheme (4.6) conserve the local proportion of atoms of different kinds. The study will be done on the model of air we used in Chapter 4 without any loss of generality.

To begin with, let us recall (4.6)

$$\left(I - \Delta t \frac{\partial \Omega}{\partial W}({W_j}^n)\right) \delta W_j = \lambda \Delta {\mathcal{F}^n}_{j+1/2} \; + \; \Delta t {\Omega^n}_j \tag{A.1}$$

To simplify the notations, let us define two linear forms ψ_1 and ψ_2 : for any $X = (x_1, x_2, x_3, x_4, x_5, x_6, x_7)$,

$$\psi_1(X) = \frac{x_1}{m_1} + \frac{x_3}{m_3} + 2\,\frac{x_4}{m_4}$$
$$\psi_2(X) = \frac{x_2}{m_2} + \frac{x_3}{m_3} + 2\,\frac{x_5}{m_5}$$

At time t^n, we have

$$\alpha \left[\frac{{\rho_1}^n}{m_1} + \frac{{\rho_3}^n}{m_3} + \frac{{\rho_4}^n}{m_4}\right] = \beta \left[\frac{{\rho_2}^n}{m_2} + \frac{{\rho_3}^n}{m_3} + \frac{{\rho_5}^n}{m_5}\right] \tag{A.2}$$

(for air, $\alpha = 21$ and $\beta = 79$)

This relation may be rewritten as (W^n is the state of the system at time t^n)

$$\alpha \psi_1(W^n) = \beta \psi_2(W^n) \tag{A.3}$$

We have to show the same relation at time t^{n+1}.

First of all, we have to notice once again that :

$$\psi_1(\Omega) = 0$$
$$\psi_2(\Omega) = 0$$

Hence we just have to show that

$$\alpha\psi_1\left(\Delta\mathcal{F}_{i+1/2}{}^n\right) = \beta\psi_2\left(\Delta\mathcal{F}_{i+1/2}{}^n\right) \ . \tag{A.4}$$

Since $\mathcal{F}^n{}_{i+1/2} = \frac{1}{2}\left[F(W^n{}_i) + F(W^n{}_{i+1}) - \mid \bar{A} \mid \Delta W^n\right]$, since $\psi_k(F(W_i)) = \psi_k(W)u$, $k = 1, 2$ (u is the velocity) and since, by definition, W_i and W_{i+1} verify (A.3), we just have to show :

$$\alpha\psi_1(\mid \bar{A} \mid \Delta W) = \beta\psi_2(\mid \bar{A} \mid \Delta W) \tag{A.5}$$

Now, by definition ($(R_i)_{i=1,7}$ are the eigenvectors of $\bar{A}$)

$$\Delta W = \sum_{i=1}^{7} \theta_i(\Delta W)R_i$$

Then,

$$\mid \bar{A} \mid \Delta W = \phi(\bar{u})\sum_{i=1}^{n.s} \theta_i(\Delta W)R_i + \phi(\bar{u} - \bar{a})\theta_6(\Delta W)R_6 + \phi(\bar{u} + \bar{a})\theta_7(\Delta W)R_7$$

where $\phi(x) \equiv \mid x \mid$ or any function of x which enable to take into accounts entropy corrections for Roe's flux. The expressions of R_i and $\theta_i(W)$ are :

$$[R_1, \ldots, R_7] = \begin{pmatrix} 1 & 0 & \ldots & 0 & \bar{Y}_1 & \bar{Y}_1 \\ 0 & 1 & \ddots & 0 & \bar{Y}_2 & \bar{Y}_2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & \bar{Y}_5 & \bar{Y}_5 \\ \bar{u} & \bar{u} & \ldots & \bar{u} & \bar{u} - \bar{a} & \bar{u} + \bar{a} \\ \frac{\bar{u}^2}{2} - \frac{\bar{\chi}_1}{\bar{\kappa}} & \frac{\bar{u}^2}{2} - \frac{\bar{\chi}_2}{\bar{\kappa}} & \ldots & \frac{\bar{u}^2}{2} - \frac{\bar{\chi}_5}{\bar{\kappa}} & \bar{H} - \bar{u}\,\bar{a} & \bar{H} + \bar{u}\,\bar{a} \end{pmatrix}$$

and

$$\begin{aligned}
\theta_1(W) &= \Delta\rho_1 - \bar{Y}_1\mathcal{A} \\
&\vdots \\
\theta_5(W) &= \Delta\rho_5 - \bar{Y}_5\mathcal{A} \\
\theta_6(W) &= \tfrac{1}{2}(\mathcal{A} - \mathcal{B}) \\
\theta_7(W) &= \tfrac{1}{2}(\mathcal{A} + \mathcal{B})
\end{aligned}$$

where $\mathcal{A}$ and $\mathcal{B}$ are functions of the averaged velocity, pressure, speed of sound, etc. We do not give the precise values of $\mathcal{A}$ and $\mathcal{B}$ since it is of no use in the present context. They can be found in Yee [4] for example.

Now, if $\Xi = (\Delta\rho_1, \ldots, \Delta\rho_5, 0, 0)$ and $\bar{Y} = \left(\bar{Y}_1, \ldots, \bar{Y}_5, 0, 0\right)$, we have :

$$\begin{aligned}
\psi_k(|\,\bar{A}\,|\Delta W) &= \phi(\bar{u})\psi_k(\Xi) - \phi(\bar{u})\,\mathcal{A}\,\psi_k(\bar{Y}) \\
&+\phi(\bar{u}-\bar{a})\frac{\mathcal{A}-\mathcal{B}}{2}\psi_k(\bar{Y}) + \phi(\bar{u}+\bar{a})\frac{\mathcal{A}+\mathcal{B}}{2}\psi_k(\bar{Y}) \quad k = 1, 2
\end{aligned}$$

Since (A.3) is true for W_i and W_{i+1}, since the ψ_k's are linear, then (A.5) holds.

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Imprimé en France
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